TECHNICAL MEMORANDUM #5: RECOMMENDATIONS FOR NUMERICAL MODEL DEVELOPMENT

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Prepared for
Regional Water Quality Control Board
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1 BACKGROUND

The relationship between selenium loads entering the North San Francisco Bay (NSFB) and the resulting concentrations in water, sediments, and biota will be represented using a mathematical model. The key question to be addressed through a modeling framework, widely used in TMDL studies, is the estimation of concentrations that might result from different combinations of loads, and can be used to determine load allocations that are consistent with numeric targets that have been adopted for the TMDL. The proposed model can be used to represent the linkage between external and internal sources of selenium, resulting water quality in the bay, and potential concentrations in organisms of interest, including primary producers and higher trophic level organisms. This technical memorandum (TM-5) presents an overview of published models and provides a recommendation for the approach that could be used for the selenium TMDL in NSFB. Additional details on the modeling to be performed, including the specific formulations used for the transport and biogeochemical processes and specific scenarios to be evaluated will be presented in TM-6.

Physical and geochemical processes have been studied through modeling in San Francisco Bay over the last two decades. Published studies have been related to hydrodynamics and salinity (Casulli and Cheng, 1992; Cheng et al., 1993; Uncles and Peterson, 1995; Gross et al., 1999; Cheng and Casulli, 2001), real-time modeling of the movement of spilled contaminants in the bay through tidal action (NOWCAST system, Cheng and Smith, 1998), sediments (McDonald and Cheng, 1997), and fate and transport of PCBs (Oram et al., 2008). Besides these, two recently published mathematical models of selenium in San Francisco Bay have also been developed (Presser and Luoma, 2006; and Meseck and Cutter, 2006).

In this document, the selenium and PCB models are discussed in some detail because of their relevance for the TMDL. These models have the benefit of being peer-reviewed, easily accessible, and contain a synthesis of the extensive research knowledge from some of the largest selenium programs in the bay. For completeness, this discussion also presents the EFDC model, a general three-dimensional hydrodynamics and water quality model that has been widely applied for pollutant transport in estuaries. Although not employed for selenium transport, this model was considered as an alternative to the more hydrodynamically simplified Meseck and Cutter (2006) and Presser and Luoma (2006) approaches.

2 EXISTING MODELS FOR APPLICATION IN THE NORTH SAN FRANCISCO BAY SELENIUM TMDL

2.1 PRESSER AND LUOMA MODEL (2006)

The Presser and Luoma model conceptualizes the fate of selenium under various loading scenarios, with an emphasis on sources from the Central Valley, including the San Joaquin River, the Sacramento River, and from petroleum refineries. The specific objective of the study was to evaluate the effect of various levels of selenium discharge from San Joaquin Valley through the proposed San Luis Drain. Since the publication of this report, the San Luis Drain is no longer an option for disposal of selenium from San Joaquin Valley (U.S. Department of Interior, 2007); however the model framework, including the load calculation and the bioaccumulation to higher trophic level organisms, is still applicable.

Figure 2-1 shows the Presser and Luoma (2006) conceptual model representing the processes of selenium bioaccumulation. The conceptual model focuses on predicting the composite freshwater concentration at the head of the bay for individual selenium species. From this predicted concentration, predictions in phytoplankton, algae, bed sediment, prey (such as clams), and predators (such as sturgeon and diving ducks) are made.

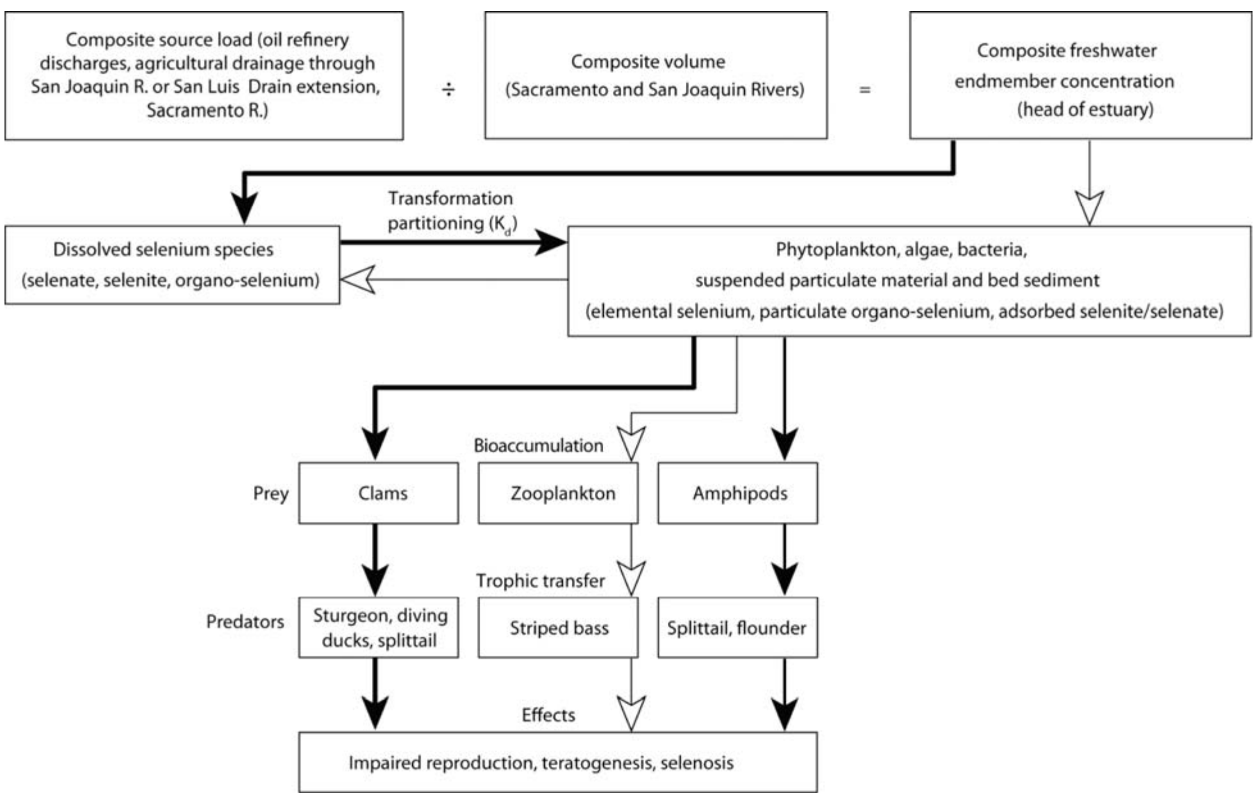

Figure 2-1 Conceptual model describing linked factors that determine the effects of selenium on ecosystems. (from Presser and Luoma, 2006)

Presser and Luoma describe a model (DYMBAM for Dynamic Bioaccumulation Model) that was used to make some of the calculations. Some predictions provided by Presser and Luoma are shown here to illustrate the capabilities of the model. The analyses presented here assume that loads from the San Luis Drain are absent, a factor not of immediate interest to the calculations because of the rejection of this alternative by the U.S. Department of the Interior (2007). For more details on DYMBAM, see Appendix A.

Five related tables that follow are abbreviated from Presser and Luoma, and each table illustrates separate but related issues. Table 2-1 shows pre-refinery cleanup scenarios (consistent with loading from refineries prior to the late 1990's) for a wet year (1997) and a critically dry year (1994). Total water column concentrations of selenium were predicted at two locations: the freshwater endpoint at the head of the estuary (the term *freshwater end member* is used for this location in Presser and Luoma (2006)), and at Carquinez Strait. The freshwater endpoint is calculated as shown previously in Figure 2-2, and the concentration at Carquinez Strait is based on decreasing the end member concentration by a known dilution based on salinity. The table shows that the low flow seasons are the most critical of the scenarios simulated. Freshwater end member concentrations vary from 0.22 μg/L to 0.53 μg/L, and concentrations at Carquinez Strait are half those values.

Table 2-2 shows post-refinery cleanup scenarios, consistent with loading from refineries prior to the late 1990's, for wet year conditions (such as 1997) and critically dry year conditions (such as 1994), with additional Central Valley Loads through San Joaquin River. Note that San Joaquin River loads as well as refinery loads are changed in this table. Total water column concentrations of selenium were predicted at two locations: the freshwater endpoint at the head of the estuary, and at Carquinez Strait. The freshwater end member is calculated as shown previously in Figure 2-1, and the concentration at Carquinez Strait is computed by reducing the end member concentration by a known dilution based on salinity. The table shows that the low flow seasons are the most critical of the scenarios simulated. Freshwater end member concentrations vary from 0.12 μg/L to 0.86 μg/L, with Carquinez Strait values calculated as above (equal to half the freshwater end member values).

Table 2-3 summarizes particulate selenium concentrations prior to refinery cleanup for three hydrologic conditions. The locations of the predictions are at the head of the estuary. For each of the three hydrologic conditions, particulate selenium concentrations are calculated using a plausible range of partition or distribution coefficients (K_d) to illustrate uncertainty. Partition coefficients represent the ratio of particulate concentrations to water column concentrations, and are commonly expressed in units of L/kg. In these examples, the concept of a partition coefficients is used as a surrogate of particle association of selenium, even though it is recognized that the underlying process is one of rate limited uptake and not strictly of thermodynamic equilibrium. Selenium particulate concentrations during a critically dry year are highest (e.g. 5.3 μg/g dry weight for a K_d of $1x10^4$ L/kg).

Predicted concentrations in bivalves for conditions prior to refinery clean-up in the 1990's are shown in Table 2-4. All predictions are at the head of the estuary. Multiple predictions for each hydrologic scenario are made to reflect uncertainties in partition coefficients and in assimilative efficiency (AE) derived from different assumptions of species composition. The predicted selenium concentrations in bivalves vary dramatically depending on data used (such as partition coefficients and assimilative efficiency) to make the predictions. For example, for predictions for a critically dry year during low flow conditions, bivalve selenium concentrations are predicted to vary from 2.3 μg/g to 53 μg/g. Table 2-5 shows results for a critically dry year that includes predictions for white sturgeon and scaup liver concentrations. The liver concentrations are based on extrapolations from regressions between bivalve and predator concentrations. For the conditions simulated, the guideline concentrations are exceeded by a factor of two to three for white sturgeon and by a factor of three to five for scaup.

A summary of the selenium loadings and calculated concentrations shown previously in Tables 2-1 through 2-5 is shown in Table 2-6. Note particularly that the predicted particulate selenium concentrations in bivalves have a large range, indicative of the uncertainties in the parameters representing bioaccumulation.

Table 2-1
Calculation of selenium concentrations for a composite freshwater end member at the head of the estuary and at Carquinez Strait (a point midway in the North Bay at a salinity of 17.5 practical salinity units) under conditions simulating those prior to refinery cleanup in 1990s. (Inputs are from the Sacramento River, San Joaquin River, and oil refineries, with no input from a San Luis Drain extension. Forecasts contrast wet and dry years; and high and low flow seasons) (modified from Presser and Luoma (2006); Table 18)

Source	Volume (million acre-ft)	Volume (billion liters)	Selenium				
			Concentration (µg/L)	Load (billion µg)	Load (lbs per six months)	Freshwater endmember (µg/L)	Carquinez Strait (µg/L)
Wet year (1997 data), high flow season (six months, December through May)							
Sacramento River	17	20,961	0.04	838	1,850		
San Joaquin River	3	3,699	1	3,699	8,160		
San Luis Drain	0	0	0	0	0		
Refineries	0.005	6	150	925	2,040		
						0.22	0.11
Wet year (1997 data), low flow season (six months, June through November)							
Sacramento River	2.3	2,836	0.04	113	250		
San Joaquin River	0.1	123	1	123	272		
San Luis Drain	0	0	0	0	0		
Refineries	0.005	6	150	925	2,040		
						0.39	0.20
Critically dry year (1994 data), low flow season (six months, June through November)							
Sacramento River	1.62	1,998	0.04	80	176		
San Joaquin River	0.1	123	1	123	272		
San Luis Drain	0	0	0	0	0		
Refineries	0.005	6	150	925	2,040		
						0.53	0.27

Table 2-2
Forecasts of selenium concentrations for a composite freshwater end member at the head of the estuary and at Carquinez Strait (a point midway in the North Bay at a salinity of 17.5 practical salinity units) for a wet year and critically dry year under load scenarios for conveyance of agricultural drainage through the San Joaquin River and refinery cleanup in the 1990s. (modified from Presser and Luoma (2006); Tables 19-21)

Source	Volume (million acre-ft)	Volume (billion liters)	Selenium				
			Concentration (g/L)	Load (billion µg)	Load (lbs per six months)	Freshwater endmember (µg/L)	Carquinez Strait (µg/L)
Wet year (1997 data); high flow season (six months, December through May); refinery cleanup							
Load scenario: Targeted San Joaquin River load of 7,180 lbs annually (3,590 lbs per six months); refinery cleanup							
Sacramento River	17	20,961	0.04	838	1,850		
San Joaquin River	1.1	1,356	1.2	1,628	3,590		
San Luis Drain	0	0	0	0	0		
Refineries	0.005	6	50	308	680		
						0.12	0.06
Wet year (1997 data); low flow season (six months, June through November); refinery cleanup							
Load scenario: Targeted San Joaquin River load of 7,180 lbs annually (3,590 lbs per six months); refinery cleanup							
Sacramento River	2.3	2,836	0.04	113	250		
San Joaquin River	0.5	616	2.5	1,541	3,400		
San Luis Drain	0	0	0	0	0		
Refineries	0.005	6.2	50	308	680		
						0.57	0.28
Critically dry year (1994); low flow season (six months, June through November); refinery cleanup							
Load scenario: Targeted San Joaquin River load of 6,800 lbs annually (3,400 lbs per six months); refinery cleanup							
Sacramento River	1.3	1,603	0.04	64	141		
San Joaquin River	0.5	616	2.5	1,541	3,400		
San Luis Drain	0	0	0	0	0		
Refineries	0.005	6.2	50	308	680		
						0.86	0.43

Table 2-3
Forecasts of selenium concentrations in a composite freshwater end member and in particulate matter at the head of the estuary under conditions prior to refinery cleanup in the 1990s. (modified from Presser and Luoma (2006); Table 25)

Climatic conditions	Composite fresh-water endmember selenium (µg/L)	Particulate selenium (µg/g dry weight)		
		($K_d=1\times10^3$)*	($K_d=3\times10^3$)*	($K_d=1\times10^4$)*
San Joaquin River targeted load of 3,590 lbs per six months for a high flow season (1.2 µg/L selenium); 3,400 lbs per six months for a low flow season (2.5 µg/L selenium)				
Wet Year/ High Flow	0.12	0.12	0.36	1.2
Wet Year/ Low Flow	0.57	0.57	1.71	5.7
Critically Dry Year/ Low Flow	0.86	0.86	2.58	8.6
Conditions prior to refinery cleanup (see Table 2-1)				
WetYear/ High Flow (1997)	0.22	0.22	0.66	2.2
Wet Year/ Low Flow (1997)	0.39	0.39	1.2	3.9
Critically Dry Year/ Low Flow (1994)	0.53	0.53	1.6	5.3

*Units of K_d (partition coefficients) are L/kg

Table 2-4
Summary of forecasts of selenium concentrations in a generic bivalve at the head of the estuary prior to refinery cleanup in the 1990s. (modified from Presser & Luoma, 2006; Table 28)

[C1 = K_d of 1×10^4, typical of suspended sediment; C2 = K_d of 3 x 10^3, typical of shallow-water bed sediment; ****
C3 = K_d of 1 x 10^3, typical of inefficient transformation. AE4 = 0.8; AE3 = 0.63; AE2 = 0.55; and AE1 = 0.35.]

Scenario	Particulate selenium/bivalve selenium (µg/g dry weight)
Wet year during high flow season	
C1 and AE4	2.2/22
C1 and AE3	2.2/17
C2 and AE2	0.66/4.5
C3 and AE1	0.22/0.96
Wet year during low flow season	
C1 and AE4	3.9/39
C1 and AE3	3.9/31
C2 and AE2	1.2/8.0
C3 and AE1	0.39/1.7
Critically dry year during low flow season	
C1 and AE4	5.3/53
C1 and AE3	5.3/42
C2 and AE2	1.6/11
C3 and AE1	0.53/2.3

*Units of K_d (partition coefficient): L/kg
Units of AE (assimilative efficiency): dimensionless

Table 2-5
Risk guidelines and forecasts of selenium concentrations in water, particulate material, a generic bivalve, scaup, and sturgeon at the head of the estuary prior to refinery cleanup in the 1990s. (modified from Presser & Luoma, 2006; Table 33)

[Forecasted predator liver concentrations are predicted by extrapolation from regressions between bivalve and predator concentrations using data from 1986 to 1990 . C2 = K_d of 3 × 10^3, typical of shallow-water bed sediment. AE2 = 0.55]

Critically dry year, low flow season				
Selenium				
Composite freshwater endmember (µg/L)	Particulate (µg/g dry weight) C2 = K_d of 3×10^3	Bivalve (µg/g dry weight) AE2 = 0.55	White sturgeon liver (µg/g dry weight)	Greater and lesser scaup liver (µg/g dry weight)
Conditions prior to refinery cleanup				
0.53	1.6	11	30	65
Guidelines*				
1–5	0.4–1.5	2–5	12–15	10–18

*Guidelines are used here as reference points for context (Presser and Luoma, 2006).

Table 2-6
Summary of Selenium Loadings and Calculated Concentrations for Selected Cases Examined from Presser and Luoma (2006) for North San Francisco Bay

Scenario	Sacramento River, kg	San Joaquin River, kg	Refineries, kg	Other Local Sources	Freshwater End Member Total Selenium Concentration, µg/L	Carquinez Strait Total Selenium Concentration, µg/L	Particulate Selenium at Head of Estuary, µg/g	Selenium Bivalve Concentrations, µg/g
1997 high flow season (6 months)	1850	8160	2040	0	0.22	0.11	0.22-2.2	1-22
1997 low flow season (6 months)	250	270	2040	0	0.39	0.2	0.39-3.9	1.7-39
1994 critically dry season (6 months)	180	270	2040	0	0.53	0.27	0.53-5.3	2.3-53
1997 high flow season with targeted loads (6 months)	1850	3600	680	0	0.12	0.06	0.12-1.2	Not Calculated
1997 low flow season with targeted loads (6 months)	250	3400	680	0	0.57	0.28	0.57-5.7	Not Calculated
1994 critically dry season with targeted loads (6 months)	140	3400	680	0	0.86	0.43	0.86-8.6	Not Calculated

The Presser and Luoma conceptual model and bioaccumulation model DYMBAM provide one method for translating selenium loads from the San Francisco Bay Delta and petroleum refineries into concentrations in the environment, including in prey and predator species (from bivalves to water fowl or fish). It is worthwhile to summarize the major assumptions in this method to understand its capabilities and limitations:

- The model, as applied in Presser and Luoma's report is steady-state, although a dynamic version of the model is also discussed there. Calculations are performed for specific periods, but the transitions between these periods, in water column or tissue concentrations, are not addressed.
- The model considers selenium sources from the Sacramento and San Joaquin Rivers, the San Luis Drain, and petroleum refineries. Local tributary loadings are not included, but could be added.
- All sources are lumped together at a single location (freshwater end member) and concentrations are calculated representative of this location. Concentration estimates at other locations in North San Francisco Bay are based on dilution estimated from salinity profiles.
- The exchange between particulate and dissolved phases of selenium is conceptualized as an equilibrium partition, and represented as a partition coefficient, although it is understood that the particle concentrations are the result of active uptake and not thermodynamic equilibrium. Equilibrium partition coefficient pertains to total dissolved selenium, and not to a particular species.
- Observed data are used to develop regression analyses to relate concentration in prey (such as bivalves) to concentrations in predators (such as waterfowl).
- Growth rates of predators are neglected in the examples shown.
- The bioaccumulation pathway in DYMBAM focuses on bivalves as the single prey. The pathways shown in Figure 2-2 that begin with zooplankton and amphipods are not included.

2.2 MESECK AND CUTTER MODEL OF SELENIUM IN SAN FRANCISCO BAY

The Meseck and Cutter (2006) model represents the chemistry of selenium in NSFB and considers freshwater and tidal mixing through a one-dimensional estuarine model, but does not consider bioaccumulation beyond primary producers. The model was implemented in a general estuary modeling framework called ECoS (Harris and Gorley, 2003). The model includes the capability to predict selenium speciation and has been calibrated and validated against data collected during high and low flow.

The representation of selenium transformation processes is shown in Figure 2-3. Mass loadings are assumed to be from refinery effluents and the Sacramento and San Joaquin Rivers. Advective and diffusive transport move selenium throughout the bay. Bed exchange occurs through particle settling and through biotic uptake. Both biotic and abiotic reactions facilitate transformations of selenium between species, and influence uptake by primary producers. Dissolved and particulate species in Figure 2-3 are identified by the letters "d" and "p" respectively. In the water column, particulate organic selenium (p Org Se(-II)) undergoes regeneration to form dissolved organic selenium (d Org Se(-II)), which can be oxidized to selenite (d Se(IV)) relatively quickly and further to selenate (d Se (VI)). Similar transformations can occur in sediment porewater. In sediment, particulate elemental selenium (p Se(0)) is formed through microbial dissimilatory reduction. Trophic transfer occurs to consumer organisms such as bivalves. The Meseck and Cutter conceptual model does not consider selenium uptake by predators, such as waterfowl, that consume bivalves and also does not simulate volatilization by methylated selenium.

Total particulate selenium, is defined as the sum of particulate elemental selenium, adsorbed selenite plus selenate, and organic selenide. It is derived from sediment resuspension, sediment loading from the Sacramento River, and in situ production (e.g., phytoplankton uptake of selenium). In bedded sediments, particulate selenium can undergo oxidation-reduction reactions that can cause the selenium to be mobilized or buried.

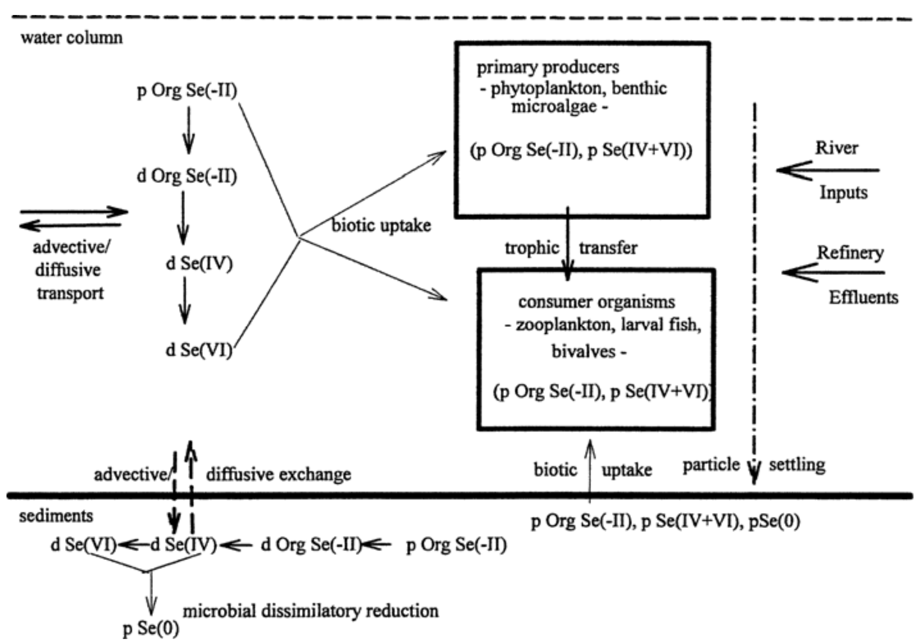

Figure 2-2 Conceptual diagram of selenium's biogeochemical cycle in the San Francisco Bay estuary, with the major chemical speciation of particulate selenium in primary producers and consumer organisms indicated in brackets. Arrows represent fluxes or transformations; p is particulate and d is dissolved. (from Meseck and Cutter (2006))

A few results from the Meseck and Cutter work illustrate the predicted distribution and behavior of selenium in the bay. Figure 2-3 shows predictions of dissolved and particulate selenium for a high flow month (April) and a low flow month (November) for a range of refinery loadings. The salinity is a surrogate for distance from the Delta to the Golden Gate. The loadings correspond to these three discharge scenarios: zero refinery inputs; 38 moles/day (1100 kg/yr), to represent conditions after cleanup; and 99 moles/day (2900 kg/yr) to represent conditions before cleanup. Note that these load estimates are higher than what is now estimated for refineries (Presser and Luoma, 2006; TM-2).

Dissolved selenium concentrations for high flow conditions calculated using this model (Figure 2-3a and Figure 2-3b) show the progressive decrease in response to loading reductions for both conditions. The mid-estuary peak is reflective of the local discharges, and diminishes as refinery loads decrease. The particulate concentrations (Figure 2-3c and Figure 2-3d) are less responsive to refinery load changes.

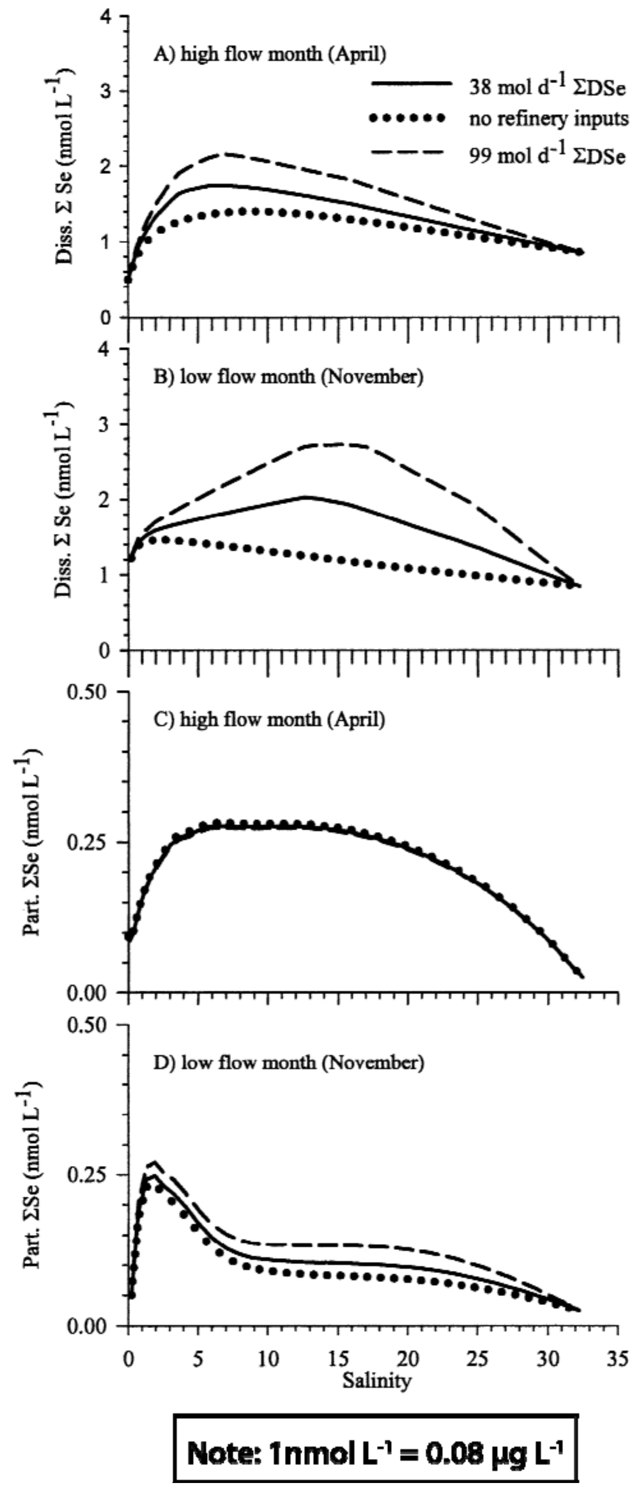

Figure 2-3 Estuary response to loading charges.(A) Model predictions for total dissolved selenium during a high flow month and (B) a low flow month and (C) total particulate selenium for a low flow month and (D) a high flow month in the San Francisco Bay under varying refinery discharge rates.

Selenium was speciated as: 13% selenite, 57% selenate, and 30% organic selenide (from Meseck and Cutter, 2006).

Several model predictions are compared against observed data to evaluate the performance of the model (Table 2-7). The range of predicted and observed data represent concentration changes along the salinity gradient, and generally agree with each other. Additional details on model calibration, validation, and sensitivity analysis are presented in Meseck (2002).

Table 2-7
Comparison of predictions and observations from Meseck and Cutter (2006) model

	Total dissolved (µg/L)-Predicted		Observed Data	
	Range	Average	Range	Average
April 1986 high flow	0.08-0.24	0.16	0.09-0.24	0.16
June 1998 high flow	0.08-0.24	0.16	0.12-0.30	0.19
April 1986 low flow	0.08-0.24	0.16	0.13-0.28	0.2
Oct. 1998 low flow	0.08-0.16	0.12	0.08-0.12	0.12
	Particulate (µg/L)			
June 1998 high flow	0-0.02	0.01	0-0.02	0.01
Oct. 1998 low flow	0-0.02	0.01	0-0.015	0.01

2.3 Multi-Box PCB Model

Although PCBs behave differently from selenium, the PCB model being developed in the bay has some features of relevance to the selenium TMDL, in particular the use of a multi-box spatially distributed approach for modeling, and its use in a TMDL over the larger water body under investigation (the entire San Francisco Bay is represented). Key features of this model are thus discussed here.

The multi-box model of polychlorinated biphenyls (PCBs) is developed around a tidally-averaged hydrodynamic model previously developed by Uncles and Peterson (1995, 1996) and widely applied in the bay (Oram et al., 2008). The salinity model employs a box-model approach, defining the bay as 50 laterally-averaged segments divided into two layers for a total of 100 boxes. In each segment, an upper box, encompassing the shallows, overlies a bottom box that extends to the deepest part of the channel in each segment. The boxes are assumed to be uniformly mixed. The multibox model includes a sediment transport model developed by Lionberger (2003). In addition to the hydrodynamic and sediment transport processes, the model incorporates fate and transport processes specific to PCBs, and includes processes such as partitioning to solids, volatilization, and degradation. Various sources of PCBS, such as the Central Valley, the tributaries, point sources, and atmospheric deposition are considered.

The model outputs in sediment PCB concentrations for different locations are compared with data in Figure 2-4. The general trend in the sediment reflects the historical loads of PCBs to the bay, and is consistent with observed data, although the uncertainties in the model predictions are significant.

The PCB model has been used to describe long-term trends in total PCB concentrations in the water column and bed sediment and to estimate timescales of recovery with respect to water quality impairment by PCBs. Because historical sources to San Francisco Bay are known only approximately, the model has been applied in hindcast mode to compare with historical patterns in loading. The model has also been applied in forecast mode to evaluate PCB concentrations in the bay under different loading scenarios.

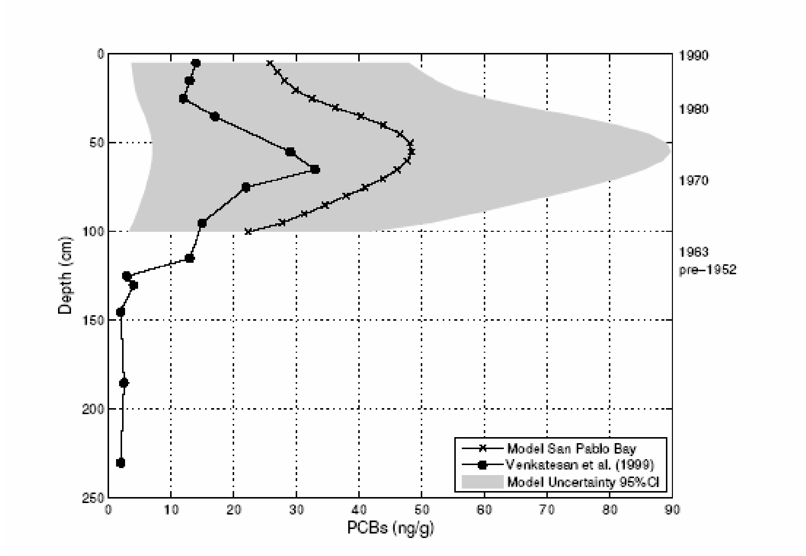

Figure 2-4 Calibrated hindcast model results of the vertical profile of in bed sediments compared to data from the bay (core obtained from San Pablo Bay). The gray shaded area reflects the uncertainty in model predictions. Source: Oram et al., 2008.

2.4 EFDC MODEL

The EFDC model is a three-dimensional hydrodynamic and water quality model (Hamrick, 1992) applied widely in the study of estuarine contaminant fate and transport.

EFDC can simulate water and water quality constituent transport in geometrically and dynamically complex water bodies, such as vertically mixed shallow estuaries, lakes, and coastal areas. The EFDC model solves the three-dimensional, vertically hydrostatic, free surface, turbulent averaged equations of motion for a variable density fluid. Dynamically coupled transport equations for turbulent kinetic energy, turbulent length scale, salinity and temperature are also solved.

The EFDC model also simultaneously solves transport-transformation equations for dissolved and suspended materials. For example, equations describing the transport of suspended sediment, toxic contaminants, and water quality state variables are also solved. Multiple size classes of cohesive and noncohesive sediments and associated deposition and resuspension processes and bed geomechanics are simulated. The model also allows for drying and wetting in shallow areas by a mass conservative scheme. For near-shore surf zone simulation, the EFDC model can incorporate externally specified radiation stresses due to high frequency surface gravity waves. Externally specified wave dissipation due to wave breaking and bottom friction can also be incorporated in the turbulence closure model as source terms. For the simulation of flow in vegetated environments, the EFDC model incorporates both two and three-dimensional vegetation resistance formulations (Hamrick and Moustafa, 1995).

3 Desirable attributes of a model that could be used for the North San Francisco Bay Selenium TMDL

Specific characteristics of a fate and transport model that may be appropriate for the North San Francisco Bay TMDL are listed, and briefly discussed. They are:

- The model should allow examination of different hydrologic conditions associated with wet and dry seasons. Critically dry seasons especially should be evaluated. The model should step forward in time at intervals that are short compared to seasons.
- The model should be able to make predictions that vary not only over time, but over space as well. For example, mid-estuary selenium sources could generate local selenium maxima in the water column and/or biota.
- The model should consider the different uptake rates for different selenium species. Due to the much higher uptake rate of selenite and selenide than selenate to particulates, it will be important to reflect this in the modeling work.
- The model should consider uptake by higher trophic levels beyond the primary producers, i.e., from algae to bivalves, and to predator species. This is because the final numeric targets may be based on concentrations in biota, rather than in the water column or sediments.

4 MODEL RECOMMENDATION

Because of the diverse range of factors that influence selenium cycling in North San Francisco Bay, it is not appropriate to treat the bay as a homogeneous system which exerts a uniform ecological risk to predators. Rather, due to the variety of point and nonpoint sources, their discharge temporal variability (dry and wet seasons), and the bioavailability of selenium associated with each source, potential impacts could be manifested locally, such as near tributaries that discharge selenium at high concentrations, in wetlands, or near outfalls. Seasonality of impacts may vary as well, based on when critical life-cycle stages are present. For this reason, a model that reflects spatial variability in the bay due to varying freshwater inflows with seasons is recommended. The salinity correction approach used by Presser and Luoma (2006) is one possibility, although the Meseck and Cutter (2006) approach is more mechanistically detailed, and builds on the tidally-averaged model developed by Uncles and Peterson (1995). The latter framework, including the software tool used to build the model, ECoS (Harris and Gorley, 2003), is recommended for this application, particularly to compute selenium speciation in the dissolved and particulate phases.

The conceptual model DYMBAM discussed and applied in Presser and Luoma (2006) was the only quantitative tool for the bioaccumulation of selenium up the food chain from prey to predator that has been applied to North San Francisco Bay. It is recommended that this model be embedded in the Meseck and Cutter (2006) representation of fate and transport to provide a composite tool that links sources to biological endpoints. The bioaccumulation part of the model will use the dissolved and particulate selenium concentrations in different locations in the bay as a starting point and use the latter to calculate concentrations in bivalves as used in Presser and Luoma (2006). Bivalve concentrations will be used for estimating concentrations in predator species (either whole body or specific organs) using regression-type relationships developed from data. Details of these steps will be presented in TM-6.

Given the episodic and spatially limited nature of selenium sampling, compared to other parameters such as salinity or currents, a spatial representation more detailed than the one-dimensional approach used in the Meseck and Cutter (2006) model, such as building on the EFDC model, was not considered appropriate. Detailed three-dimensional hydrodynamic modeling is computationally intensive, and with insufficient data for calibration, there are limits to the benefits obtained from the spatially detailed representation. Further, the selenium cycling component of the model would have to be programmed specifically for this application.

The multi-box model, now under peer review and developed by Oram et al. (2008), is a possible framework for approaching the selenium modeling. However, modifying the existing tool for selenium will require additional programming effort, and may require significant new calibration and validation exercises for application to sources, fate, and transport of selenium.

In contrast to some of the tools discussed here, the Meseck and Cutter (2006) approach is built with specific selenium reactions (biotic and abiotic) and is developed for the same geographical area as required by the TMDL. The model has been calibrated and validated using data in NSFB, and includes estimates of key parameters. The underlying salinity model (Uncles and Peterson, 1995) is the same as that employed by Oram et al. (2008). The model has been peer reviewed and the computer program developed to run it is available. However, the model does not include bioaccumulation processes which are expected to be very important for the selenium TMDL.

Based on the above discussion, it is our recommendation that model calibration and validation efforts for the TMDL should build on the earlier work by Meseck and Cutter (2006) for water column chemistry and by Presser and Luoma (2006) for bioaccumulation. As described in TM-2, detailed selenium speciation data exist in the bay for the following years: 1986, 1997, 1998 and 1999. However there are other selenium data for subsequent years collected through the RMP efforts, but these do not contain speciation information. Because the interest in this TMDL is on future scenarios following refinery waster treatment improvements in 1998, it is proposed that the model be calibrated to 1999 conditions and validated against RMP total selenium data for 2001 and 2005. The validation will reflect hydrologic variability in the system: 1999 was an average rainfall year, whereas 2001 was a dry year, and 2005 was a wet year. For future application of the model, where the responses are characterized for different influent loads, hydrological conditions representing these three years can be used for comparing different loading scenarios.

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Appendix A
Background Application of Presser-Luoma Model DYMBAM

Introduction

- Developed by Presser and Luoma (2006) to model Se bioaccumulation in the Bay-Delta
- The model is applied in a steady-state mode, although a dynamic model is also presented but apparently not used.
- Their conceptual model is shown below (from USGS Fact Sheet 2004-3091) in Figure A-1. Selenium is discharged from both the Sacramento and San Joaquin rivers, from three alternate San Luis Drain scenarios, and from refineries. Concentrations at the freshwater endpoint are then calculated. Using partition coefficients, particulate selenium concentrations are calculated. Clams then consume particulates, and bioaccumulate the selenium. Finally, predators (fish and birds) consume clams and further bioaccumulate selenium.

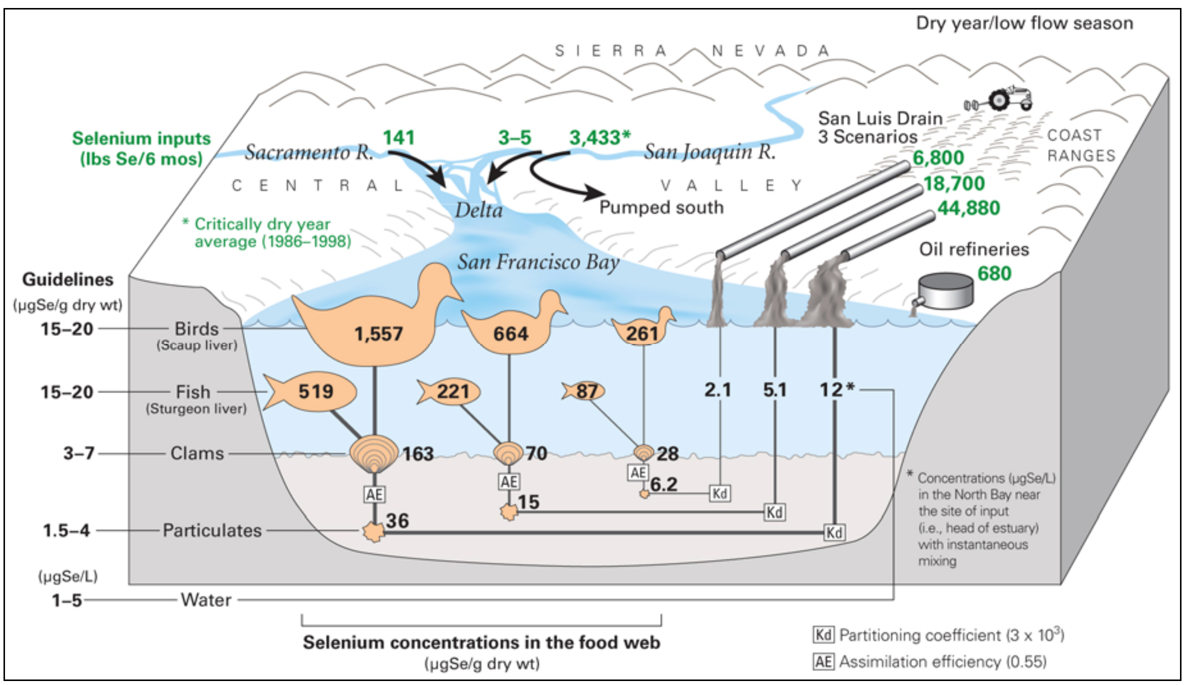

Figure A-1 Conceptual model and illustrative computations from DYMBAM

Summary of DYMBAM

- Uses experimentally established uptake rates of Se in prey (bivalves) differentiated by Se species to predict Se concentrations in prey
- Uses predicted environmental concentrations along with regression analysis to predict tissue concentrations in predators (fish and birds), once concentration in prey is forecast.

Advantages of DYMBAM Approach (as stated by Presser & Luoma)

- Bioaccumulation in bivalves can be derived for different speciation regimes that may change over time as Se loading changes
- Forecasts are verifiable by comparing with observations in tissues of resident species.
- More background on the model can be found in Luoma and Fisher (1997), Schlekat et al. (2002 a, b), and Luoma and Rainbow (2005).

DYMBAM Predicts the Following

- Se loads, water volume associated with those loads, and waterborne concentrations
- Waterborne concentrations include both freshwater endmember concentrations (concentrations at head of estuary where salinity is zero), and concentrations within the estuary (salinity dependent)
- Bioaccumulation in bivalves (prey)
- Tissue concentrations in predators (via regression analysis)
- Seasonal responses: dry/wet seasons of dry/wet years

Component Equations for DYMBAM

- Steady-state model version
- Freshwater endmember Se concentrations:

$C_{fe} = \frac{\Sigma C_i V_i}{\Sigma V_i}$ (see p38, Presser and Luoma, 2006; bulleted item)

Where
C_{fe} = freshwater endmember concentration
C_i = total Se concentration in source i, μg/L
V_i = volume associated with source i over hydrologic conditions simulated

Total selenium water column concentration at location x within estuary (see Fig 10, p39 of Presser and Luoma, 2006)

$C_x = f_x C_{fe} + (1-f_x) C_o$
where
$f_x = \frac{S_o - S_x}{S_o}$ = fraction of freshwater at x
C_o = concentration near Golden Gate
C_x = Se concentration in water column at x

Selenium concentration in particulate matter (e.g., phytoplankton, suspended particulate matter, bed sediment) (conceptually shown in Fig 2, p4 of Presser and Luoma, 2006):

$C_p = K_d \cdot C_{x,d}$

where

- K_d = distribution coefficient that relates dissolved and particulate selenium concentrations, L/g
- $C_{x,d}$ = dissolved Se concentration at location x, µg/L
- C_p = particulate Se concentration, µg/g

Tissue Concentration in Bivalve at Steady-State

$C_{m,ss} = (I_f+I_w)/(k_e+g)$ (from Eq. (1) in Presser and Luoma, 2006, p 49; time derivative set to zero)
Cm,ss = Steady-state Se concentration in tissue (of bivalves, typically),µg/g
I_f = Se influx from food
I_w = Se influx from water
k_e = rate constant for Se loss from organism, day^{-1}
g = rate of growth of organism (ignored in later developments)
I_f = (FR)(C_f)(AE) (from Eq. (5), p50)

- FR = feeding rate per gram of tissue , g-food/g-tissue/day
- C_f = concentration of Se in food (concentration in particulate matter for bivalves), µg/g
- AE = assimilative efficiency of selenium in food consumed (depends on Se speciation) or fraction of ingested selenium taken up into tissues, g-assimilated/g-intake

Operative Equation

$C_{m,ss} = [I_w + (FR \cdot C_f \cdot AE)]/k_e$ (Eq. (6), p50)

$AE = \Sigma fr_i AE_i$

$fr_i = \text{fraction of Se in species category } i \; (\Sigma fr_i = 1)$

$AE_i = \text{assimilative efficiency in category } i \; (\text{low}: AE = 0.2 (\text{low bioavailability}); \text{hi}: AE = 0.8)$

<u>Then</u> regression is used for predator concentrations, based on data such as below (p89)

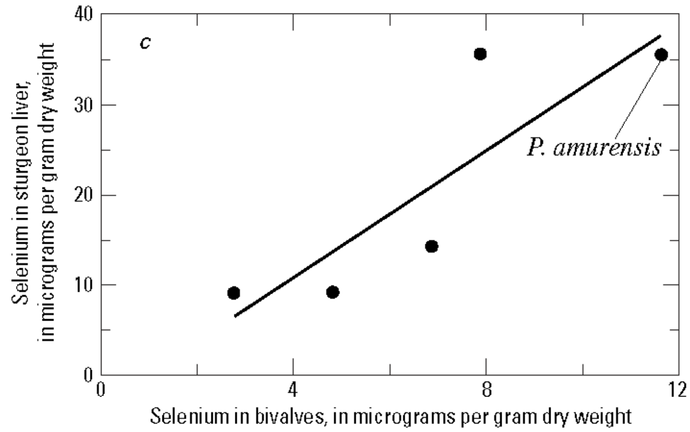

Figure A-2 Example relationship between selenium in bivalves and selenium in sturgeon liver.

Table A-1
Typical Ranges of Data used by P&L to Compute Tissue Concentration of Bi-valves (see pp. 82-83)

Variable	Range	General Importance
Iw	0-?	Unimportant: neglected
FR	0.20 – 0.27 g-food/g-tissue-day	Important
AE	0.2 - 0.8 g-assimilated/g-intake	Important
ke	0.01 – 0.03/day	Important
kg	0-?	Unimportant: neglected
Kd	10^3 – 10^4 l/kg	Important

Example Application

- Dry season of a critically dry year (1994) – see Table 18, p. 68, in Presser and Luoma, 2006
- Se discharge conditions are assumed to be prior to refinery clean-up in 1990s
- San Luis Drain not operational
- Specified concentrations and flow rates in Sacramento and San Joaquin River consistent with critically dry year
- No other sources of Se loading are considered

Example Application (cont'd)

Calculate freshwater end member concentration

$$C_{fe} = \frac{(1998 \cdot 0.04 + 123 \cdot 1 + 6 \cdot 150)}{(1998 + 123 + 6)} = 0.52\ \mu g/L \text{ (freshwater endpoint)}$$ (0.53 is shown in Table 18)

$$Cx = \frac{35 - 17.5}{35}(0.52) = 0.26\ \mu g/L, \text{at Carquinez Strait}$$ (Example at bottom of Table 18 P&L)

For $K_d = 10^4$

$Cp = K_d \cdot C_{fe} = 10^4 \cdot (0.52) \cdot 10^{-3} = 5.3\ \mu g/g$ (Example at bottom of Table 24 P&L)

For $AE = 0.8, FR = 0.25, ke = 0.02$

$C_{m,ss} = [0 + (0.25)(5.3)(0.8)/0.02] = 53\ \mu g/g$, bivalve Se concentration (Example at bottom of Table 28)

Predator Example (not used by Presser and Luoma, 2006)

Suppose $C_{m,ss} = 53\ \mu g/g$

Regression shows : $C_{sturgeon\ liver} \approx (3.15)(53) - 3.50 = 167\ \mu g/g$

(Regression coefficients from bottom half of Table 30, p 90)

- This specific example is not in Presser and Luoma, 2006. However the regression coefficients used were verified by recreating results in Table 32, p 93.